Benzene

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 1.13e-02 mol/L

Global applicability domain: Inside

Local applicability domain index: 8.06e-01

Confidence level: 8.85e-01

Nearest Neighbors from the Training Set

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Propane, 2-iodo-
Measured: 8.24e-03
Predicted: 8.51e-03

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1,2-Dibromoethane
Measured: 2.21e-02
Predicted: 1.94e-02

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Ethane, iodo-
Measured: 2.51e-02
Predicted: 2.23e-02

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1-Butanethiol
Measured: 6.62e-03
Predicted: 7.55e-03